Ising transition in a one-dimensional quarter-filled electron system with dimerization

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Abstract

We examine critical properties of the quarter-filled one-dimensional Hubbard model with dimerization and with the onsite and nearest-neighbor Coulomb repulsion U and V. By utilizing the bosonization method, it is shown that the system exhibits an Ising quantum phase transition from the Mott insulating state to the charge-ordered insulating state. It is also shown that the dielectric permittivity exhibits a strong enhancement as decreasing temperature with power-law dependence at the Ising critical point.

Key words: A. organic compounds, D. electronic structure, D. phase transitions

The Bechgaard salts $(TMTSF)_2X$ and the Fabre salts $(TMTTF)_2X$ form a family of organic conductors with quasi-one-dimensional band structure, with a long history of both theoretical and experimental research. These materials have a 3/4-filled electron (i.e., quarter-filled hole) band due to a charge transfer from two organic molecules to one counterion X. Since the transfer integral is slightly dimerized along the chain axis, the system becomes effectively half-filling. Optical and photoemission experiments on the normal states have shown evidences of a charge gap for both TMTTF salts and TMTSF salts [1,2]. This charge gap is believed to be related to the formation of a uniform insulating state. Recently, a charge ordered (CO) insulating state have been discovered by NMR measurements in the $(TMTTF)_2AsF_6$ and $(TMTTF)_2PF_6$ salts [3] and by dielectric permittivity measurements in the $(TMTTF)_2PF_6$ salt [4].

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In order to describe theoretically the insulator, one has to take into account the commensurability effect of both half-filling and quarter-filling [5]. As a simplified model, the quarter-filled one-dimensional (1D) extended Hubbard model with dimerization and with the onsite and nearest-neighbor Coulomb repulsion has been proposed and it is shown in a mean-field approach that a transition from the state with a uniform charge distribution to the CO state takes place by increasing the intersite Coulomb repulsion [6]. In order to obtain the characteristics of such a transition, the effect of quantum fluctuations must be taken into account. For this purpose, the bosonization method is applied to this system [7,8]. The model reduces to the double-frequency sine-Gordon (DSG) model for the charge degrees of freedom where two kinds of non-linear terms appear due to the half-filled and quarter-filled umklapp scattering. The DSG model has been analyzed classically [9], and quantum field theoretically [10–12,8]. In terms of the renormalization group (RG) method, it is shown that there are two-kinds of different fixed points corresponding to the Mott insulator and the CO insulator [8]. However, in the perturbative RG scheme the both fixed points are strong coupling where the perturbative RG treatment breaks down, thus the low energy states behavior and the critical behavior of the transition cannot be captured correctly.

Recently, it has been established that the critical properties of the DSG model is described as a quantum Ising transition, i.e., $c = 1/2$ CFT [10–12]. By expanding the previous analysis of the DSG model, we examine the critical properties of the quarter-filled 1D extended Hubbard model with dimerization, and also examine the physical quantities, such as dielectric response and optical conductivity, in the present study. Note that in [11,12], the related problem of the conductivity in a 1D Hubbard model with a *staggered* potential has been considered. We also discuss the experimental results on the huge enhancement of the dielectric permittivity obtained in the $(\mathrm{TMTTF})_2\mathrm{X}$ salts [4].

We consider a 1D extended Hubbard model with quarter-filling, where the corresponding Hamiltonian is given by

$$
\begin{aligned}
H = & -\sum_{j,\sigma,l} \left[t + (-1)^j t_d\right] \left(c^\dagger_{j,\sigma}\, c_{j+1,\sigma} + \mathrm{h.c.}\right) \\
& + U \sum_j n_{j,\uparrow}\, n_{j,\downarrow} + V \sum_j n_j\, n_{j+1}
\end{aligned}
\tag{1}
$$

where $n_{j,\sigma} = c^\dagger_{j,\sigma} c_{j,\sigma}$ and $c_{j,\sigma}$ denotes the annihilation operator of the electron at the j-th site with spin $\sigma(=\uparrow,\downarrow)$, and $t_d(>0)$ denotes dimerization along the chain. The onsite and nearest-neighbor Coulomb repulsions are denoted by U and V, respectively. By utilizing the bosonization method, the phase Hamiltonian is given by $H = H_c + H_s$ with [8]

$$
\begin{aligned}
H_c = & \frac{v_\rho}{4\pi} \int \mathrm{d}x \left[\frac{1}{K_\rho} \left(\partial_x \theta_+\right)^2 + K_\rho \left(\partial_x \theta_-\right)^2 \right] \\
& - \frac{g_{1/2}}{2\pi^2\alpha^2} \int \mathrm{d}x \, \sin 2\theta_+ + \frac{g_{1/4}}{2\pi^2\alpha^2} \int \mathrm{d}x \, \cos 4\theta_+,
\end{aligned} \tag{2}
$$

$$
\begin{aligned}
H_s = & \frac{v_\sigma}{4\pi} \int \mathrm{d}x \left[\frac{1}{K_\sigma} \left(\partial_x \phi_+\right)^2 + K_\sigma \left(\partial_x \phi_-\right)^2 \right] \\
& + \frac{g_s}{2\pi^2\alpha^2} \int \mathrm{d}x \, \cos 2\phi_+,
\end{aligned} \tag{3}
$$

where $\theta_\pm$ and $\phi_\pm$ are charge and spin phase variables [8] and α is a cutoff of the order of the lattice constant. In Eq. (2), the velocity and the Tomonaga-Luttinger exponent are given by $v_\rho = v_{\mathrm{F}}[(1+g_{4\rho}/2\pi v_{\mathrm{F}})^2 - (g_\rho/2\pi v_{\mathrm{F}})^2]^{1/2}$, $v_\sigma = v_{\mathrm{F}}[(1+g_{4\sigma}/2\pi v_{\mathrm{F}})^2 - (g_\sigma/2\pi v_{\mathrm{F}})^2]^{1/2}$, $K_\rho = [(2\pi v_{\mathrm{F}}+g_{4\rho}-g_\rho)/(2\pi v_{\mathrm{F}}+g_{4\rho}+g_\rho)]^{1/2}$ and $K_\sigma = [(2\pi v_{\mathrm{F}}+g_{4\sigma}-g_\sigma)/(2\pi v_{\mathrm{F}}+g_{4\sigma}+g_\sigma)]^{1/2}$. The constants g_ρ, $g_{4\rho}$, g_σ and $g_{4\sigma}$ are given by $g_\rho = g_{4\rho} = (U+4V)a$ and $g_\sigma = g_{4\sigma} = Ua$ in the lowest order of the interaction, where a is the lattice constant. The magnitude of half-filled umklapp scattering, $g_{1/2}$, and that of quarter-filled one, $g_{1/4}$, are given by [8]

$$
g_{1/4} = \frac{1}{(2\pi\alpha)^2} \frac{A^4 \, a^5}{v_{\mathrm{F}}^2} U^2 (U - 4V), \tag{4}
$$

and $g_{1/2} = BUa$ in the lowest order where $A \equiv [1-(t_d/t)^2]/[1+(t_d/t)^2]$ and $B \equiv [2t_d/t]/[1+(t_d/t)^2]$. We neglect the spin-charge coupling term $U^3 \cos 4\theta_+ \cos 2\phi_+$ due to its large scaling dimension [13]. The order parameters of the $4k_{\mathrm{F}}$ charge density wave (CDW) state and the $4k_{\mathrm{F}}$ bond ordered wave (BOW) state are given by[13]

$$
\mathcal{O}_{4k_{\mathrm{F}}\text{-CDW}}(x) \propto (-1)^{x/a} \cos 2\theta_+(x), \tag{5}
$$

$$
\mathcal{O}_{4k_{\mathrm{F}}\text{-BOW}}(x) \propto (-1)^{x/a} \sin 2\theta_+(x), \tag{6}
$$

where $k_{\mathrm{F}} = \pi/4a$.

The spin degrees of freedom becomes gapless due to the marginally irrelevance of the g_s-term. Therefore we focus hereafter on the charge degrees of freedom only. In the case of $t_d = 0$ (i.e., $g_{1/2} = 0$), it has been shown by the RG analysis that the system undergoes the Kosterlitz-Thouless transition by increasing the nearest-neighbor repulsion [13] where the gapped phase corresponds to the CO insulator. In the case of $t_d \neq 0$, the Hamiltonian H_c has two possible ground states with $\langle\theta_+\rangle = 0, \pi/2$ ($4k_F$-CDW, dominated by $g_{1/4} < 0$) or $\langle\theta_+\rangle = \pi/4$ ($4k_F$-BOW, dominated by $g_{1/2}$). These two ground states are incompatible, so we expect a phase transition of the Ising type, as discussed in [12].

By following the method of Ref. [12], we analyze the DSG model Eq. (2). By using the Jordan-Wigner transformation, the vertex operators are expressed

in terms of the order (σ_1 and σ_2) and disorder (μ_1 and μ_2) parameters of the two Ising models as follows [14,12]:

$$\sin 2\theta_+ = \sigma_1^z\,\sigma_2^z, \tag{7}$$
$$\cos 2\theta_+ = \mu_1^z\,\mu_2^z, \tag{8}$$
$$\cos 4\theta_+ = \frac{1}{2}(\sigma_1^x + \sigma_2^x). \tag{9}$$

The charge part of the Hamiltonian H_c can be expressed in terms of the quantum Ashkin-Teller model which consists of two quantum Ising spin chains coupled by a four-spin interaction term [12]:

$$H_c = H_{\rm QI}[\sigma_1,\sigma_2] + H_{\rm AT}[\sigma_1,\sigma_2] + H_h[\sigma_1,\sigma_2], \tag{10}$$

where σ_l are the Pauli matrices of l-th chain ($l = 1, 2$). In Eq. (10), $H_{\rm QI}$ is given by

$$H_{\rm QI} = -\sum_{l=1,2}\sum_n \Big[J\,\sigma_l^z(n)\,\sigma_l^z(n+1) + \Delta\,\sigma_l^x(n)\Big], \tag{11}$$

where n denotes the lattice site on the respective chain. This Hamiltonian describes two independent quantum Ising (QI) chains in a transverse magnetic field (Δ). In Eq. (10), $H_{\rm AT}$ is the Ashkin-Teller interaction term given by

$$H_{\rm AT} = J'\sum_n \Big[\sigma_1^z(n)\,\sigma_1^z(n+1)\,\sigma_2^z(n)\,\sigma_2^z(n+1) + \sigma_1^x(n)\,\sigma_2^x(n)\Big], \tag{12}$$

where this term describes a four-spin interaction. It is noted that this interaction term takes a *self-dual* form, thus this term does not make the system non-critical. Finally, H_h is a “magnetic field”-type coupling, given by

$$H_h = -h\sum_n \sigma_1^z(n)\,\sigma_2^z(n). \tag{13}$$

By using the Jordan-Wigner transformation, the parameters in Eq. (2) and those in Eq. (10) can be related as $v_\rho = 2Ja[1-(2J'/\pi J)^2]^{1/2}$, $K_\rho = (1/8)[\{1+(2J'/\pi J)\}/\{1-(2J'/\pi J)\}]^{1/2}$, $g_{1/2} = 2ah$ and $g_{1/4} = -4a(\Delta - J)$. Note that the sine-Gordon model, Eq. (2), with $K_\rho = 1/8$, $g_{1/2} = 0$ and $g_{1/4} \neq 0$, is equivalent to a model of two degenerate massive Majorana fermions, i.e., two decoupled non-critical Ising models [14], and, when the nonlinear term vanishes ($g_{1/4} \to 0$), two Ising models become critical simultaneously, i.e., critical properties are described by $c = 1$ CFT.

The origin of the Ising criticality ($c = 1/2$ CFT) in the case of $g_{1/2} \neq 0$ can be captured easily by considering the limit of large h [12]. In this case, the Ising spins are locked as $(\sigma_1, \sigma_2) = (1, 1)$ or $(-1, -1)$ where σ_i is the eigenvalue of σ_i^z. This fact implies that the "relative" degrees of freedom becomes locked (i.e., this freedom is always non-critical) while the "total" degrees of freedom asymptotically decouples and the system can become critical where the critical properties are described by $c = 1/2$ CFT. In order to analyze the physical quantities on and near the criticality, we change the basis into "total"-"relative" representation, where the relative Ising mode is described by $\tau = \sigma_1 \sigma_2$, while the total mode by e.g., $\sigma = \sigma_1$. The operator identities are given by [12]

$$
\begin{aligned}
&\sigma^z = \sigma_1^z, \qquad \tau^z = \sigma_1^z\, \sigma_2^z, \\
&\sigma^x = \sigma_1^x\, \sigma_2^x, \quad \tau^x = \sigma_2^x.
\end{aligned} \tag{14}
$$

In terms of these spin variables, Eq. (10) is rewritten as $H_c = H_\sigma + H_\tau + H_{\sigma\tau}$ where

$$
H_\sigma = \sum_n \Big[-J\, \sigma^z(n)\, \sigma^z(n+1) + J'\, \sigma^x(n) \Big], \tag{15}
$$

$$
H_\tau = \sum_n \Big[J'\, \tau^z(n)\, \tau^z(n+1) - \Delta\, \tau^x(n) - h\, \tau^z(n) \Big], \tag{16}
$$

$$
\begin{aligned}
H_{\sigma\tau} = -\sum_n \Big[&J\, \sigma^z(n)\, \sigma^z(n+1)\, \tau^z(n)\, \tau^z(n+1) \\
&+ \Delta\, \sigma^x(n)\, \tau^x(n) \Big].
\end{aligned} \tag{17}
$$

The Ising transition corresponds the situation when the σ-degrees of freedom go massless at $\Delta \approx \sqrt{h(2J + J')}$ [12]. With no regard to the Ising transition in the σ-chain, the τ-chain remains frozen in a configuration with both $\langle \tau^z \rangle$ and $\langle \tau^x \rangle$ nonzero. Here we introduce the spin variables μ and ν which are dual to σ and τ, respectively, by the Kramers-Wannier transformation: $\mu^z(n+1/2) \equiv \prod_{m=1}^{n} \sigma^x(m)$, $\mu^x(n+1/2) \equiv \sigma^z(n)\sigma^z(n+1)$, $\nu^z(n+1/2) \equiv \prod_{m=1}^{n} \tau^x(m)$ and $\nu^x(n+1/2) \equiv \tau^z(n)\tau^z(n+1)$. The spin variables μ and ν can be related with μ_1 and μ_2 by $\mu^z = \mu_1^z\, \mu_2^z$, $\mu^x = \mu_1^x$, $\nu^z = \mu_2^z$ and $\nu^x = \mu_1^x\, \mu_2^x$. The expectation value of μ^z becomes finite ($\langle \mu^z \rangle \neq 0$) in the case that σ-chain is in the disordered phase ($\langle \sigma^z \rangle = 0$), while becomes zero ($\langle \mu^z \rangle = 0$) in the ordered phase ($\langle \sigma^z \rangle \neq 0$). The order parameter of $4k_{\rm F}$-CDW is given in terms of the spin variable by $\mathcal{O}_{4k_{\rm F}\text{-CDW}} \propto \cos 2\theta_+ = \mu_1^z\, \mu_2^z = \mu^z$, and then one finds $\langle \mathcal{O}_{4k_{\rm F}\text{-CDW}} \rangle \propto \langle \mu^z \rangle \neq 0$ in the disorder phase only. Therefore the transition from the Mott insulator to the CO insulator corresponds to this order-disorder Ising quantum phase transition of the σ Ising chain, where the disordered phase of the Ising system corresponds to the CO insulating state. Note that the quantity $\langle \mathcal{O}_{4k_{\rm F}\text{-BOW}} \rangle$ takes a finite value and shows no anomaly at the

transition point, since the order parameter of $4k_{\rm F}$-BOW is given in terms of the noncritical Ising field: $\mathcal{O}_{4k_{\rm F}\text{-BOW}} \propto \sin 2\theta_+ = \sigma_1^z\,\sigma_2^z = \tau^z$.

Now we examine the dielectric permittivity and the optical conductivity at finite temperature. In the energy scale higher than the gap in the τ-chain, the perturbative analysis in terms of renormalization group method works well [8]. The complex conductivity $\sigma(\omega) = \sigma_1(\omega) + i\,\sigma_2(\omega)$ ($\sigma_1 \equiv {\rm Re}\,\sigma$ and $\sigma_2 \equiv {\rm Im}\,\sigma$) can be calculated from $\sigma(\omega) = i[\chi(\omega) - \chi(0)]/\omega$, where χ is the retarded current-current correlation function: $\chi(\omega) = -i\int dx \int_0^\infty dt \langle [j(x,t), j(0,0)]\rangle\, e^{i\omega t - \delta t}$. In terms of the complex conductivity, the dielectric permittivity is given by $\epsilon(\omega) = \epsilon_1(\omega) + i\,\epsilon_2(\omega) = 1 + (4\pi i/\omega)\,\sigma(\omega)$, where $\epsilon_1 \equiv {\rm Re}\,\epsilon$ and $\epsilon_2 \equiv {\rm Im}\,\epsilon$. By utilizing the RG method, it can be shown that the resistivity $\rho(T)$ and the dielectric permittivity $\epsilon_1(T)$ behaves as $\rho(T) = 1/\sigma_1(T) \propto T^{16K_\rho - 3}$ and $\epsilon_1(T) \propto T^{2-16K_\rho}$ in the case that the quarter-filled umklapp scattering is dominant [8]. This analysis, however, only holds in the high temperature region. In the energy scale lower than the gap in the τ-chain, we analyze these physical quantities in the quantum Ising model scheme. By using the spin variable μ, the current operator are given by [12]

$$j(x) = -\frac{1}{\pi}\,\partial_t\theta_+ \;\to -C\,\partial_t\,\mu(x), \tag{18}$$

where $\mu(x)$ is a continuum variable of $\mu^z(n)$ and and $C(\propto\,\langle\tau^z\rangle)$ is a non-universal numerical constant. Here we have used the fact that the τ-field is always non-critical and has nonzero expectation value. We introduce the response function of the Ising disorder parameter:

$$D^{(R)}(k,\omega) = -i\int dx \int_0^\infty dt\, e^{-ikx + i\omega t}\,\langle[\mu(x,t),\,\mu(0,0)]\rangle\,. \tag{19}$$

By using Eq. (18), the current-current correlation function is given by $\chi(\omega) = C^2\omega^2 D^{(R)}(0,\omega)$. Then the real and imaginary parts of the conductivity σ_1 and σ_2 are given by $\sigma_1(\omega) = -C^2\,\omega\,{\rm Im}D^{(R)}(0,\omega)$ and $\sigma_2(\omega) = C^2\,\omega\,{\rm Re}D^{(R)}(0,\omega)$. On the Ising criticality, it is known that the response function is given by $D_{\rm crit}(r) \propto 1/r^{1/4}$ where $r = (x^2 + \tau^2)^{1/2}$ with the velocity being set to unity. This power-law behavior is still valid away from the criticality in the short range region $r \ll 1/\Delta_\sigma$, where Δ_σ is the gap in the σ-part of the Ising chain. By using this asymptotic behavior, the retarded response functions is given by [14]

$$D^{(R)}_{\rm crit}(0,\omega) = -\frac{\sin(2\pi\Delta)}{(2\pi T)^{2-4\Delta}}\,B^2\left(\Delta - iS, 1 - 2\Delta\right), \tag{20}$$

where $S = \omega/4\pi T$, the conformal dimension is $\Delta(=\bar{\Delta}) = 1/16$ and $B(x,y)$ is

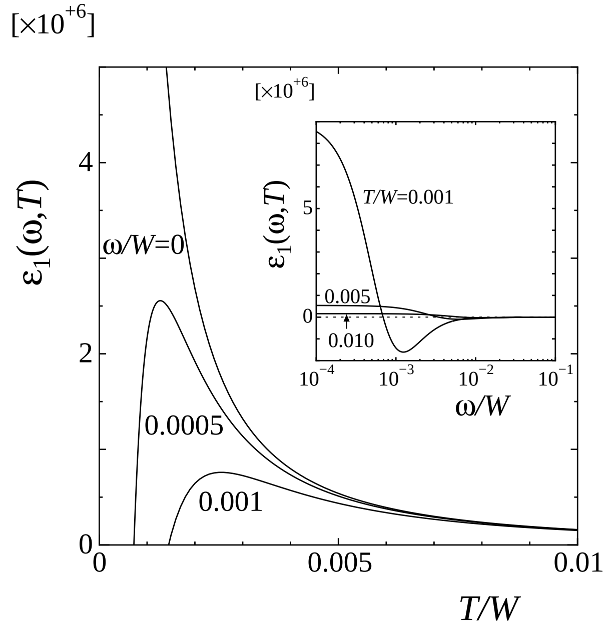

Fig. 1. The temperature dependence of the dielectric permittivity $\varepsilon_1(\omega, T)$ for $\omega/W = 0$, 0.0005 and 0.001. The inset shows the frequency dependence of $\varepsilon_1(\omega, T)$ with fixed temperature $T/W = 0.001$, 0.005 and 0.01.

the beta function given by $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$. The temperature dependence of the dielectric permittivity $\epsilon_1(\omega, T)$ with zero and finite frequency is shown in Fig. 1, where W denotes the cutoff of the order of the bandwidth and for simplicity we have set $C = 1$. The frequency dependence of $\epsilon_1(\omega, T)$ is also shown in the inset. The dielectric permittivity shows strong temperature dependence. In high temperature limit, the dielectric permittivity ϵ_1 becomes unity independent of ω, but as decreasing temperature the huge enhancement can be obtained and ϵ_1 takes a maximum at $T \approx \omega$. At low temperature ($T \lesssim \omega$), ϵ_1 decreases and changes its sign, and finally saturates to a value that depends on ω. The optical conductivity also increases as decreasing temperature, and exhibits a maximum at $T \approx \omega$. The limiting behaviors of ϵ_1 and σ_1 are given by $\epsilon_1(\omega, T) = 1 + \mathrm{const.}/T^{7/4}$ and $\sigma_1(\omega, T) \propto \omega^2/T^{11/4}$ for high temperature ($T \gg \omega$), and $\epsilon_1(\omega, T) \propto -1/\omega^{7/4}$ and $\sigma_1(\omega, T) \propto 1/\omega^{3/4}$ for low temperature ($T \ll \omega$).

Finally we discuss the experimental observation of the $(\mathrm{TMTTF})_2\mathrm{X}$ salts. Recent analysis of the dielectric response exhibits a strong temperature dependence and a huge enhancement of the dielectric permittivity as decreasing temperature [4]. In our analysis of the temperature dependence of the dielectric permittivity, we have restricted ourselves to the case on the Ising critical point. However, the results would be valid in the vicinity of the transition point in the energy region above Δ_σ. Therefore the huge enhancement could be interpreted by considering that the system is in the vicinity of the transition point from the Mott insulator to the CO insulator.

In summary, we examined the properties of the dimerized extended Hubbard model at quarter-filling in one dimension. It was shown that the phase transition from Mott insulating state to the CO insulating state in this system corresponds to the Ising quantum phase transition described by $c = 1/2$ CFT. We have also show that the dielectric permittivity exhibits a strong enhancement as decreasing temperature with power-law dependence at the Ising critical point.

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